Anomalous Behavior of the Coulomb T Matrix

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Some apparent discrepancies in the definition or calculation of the Coulomb T matrix are investigated in an approach that uses shielded wave functions. It is found that the screened Coulomb T matrix behaves anomalously in the neighborhood of the energy shell and is in fact discontinuous in the limit of zero screening. A closed-form expression for the T matrix, which has been derived previously, is shown to be essentially correct off the energy shell.

I. INTRODUCTION

IN the usual application of the impulse approximation to a many-body scattering problem, it is common to introduce the two-body scattering matrix or T matrix $(\mathbf{p}|T|\mathbf{k})$. The transition probability can then be expressed as an integral in which the T matrix is folded into the product of the initial- and final-state momentum distributions.

Usually it is necessary to make further approximations, because experimental two-body scattering data give information about the T matrix only on the energy shell $p^2 = k^2$. The most common approximation is to ignore off-the-energy-shell effects completely, putting $(\mathbf{p}|T|\mathbf{k}) \approx (k\hat{p}|T|\mathbf{k})$. However, if the two-body scattering wave function is known exactly, the T matrix can be directly calculated from the formula

$$(\mathbf{p}|T|\mathbf{k}) = \langle \Phi_p | V | \psi_k \rangle. \qquad (1)$$

Here, ψ_k is the wave function for scattering by the potential V, and Φ_p is a final-state plane wave.

Since the Coulomb wave function is known exactly in closed form, it is natural to consider using the impulse approximation for atomic scattering problems. Such calculations have been made by Pradhan,[1] for instance, in the case of electron capture by protons, and by Akerib and Borowitz[2] in the case of electron scattering by atomic hydrogen.

Recently, however, there has been some doubt that the usual formal scattering theory, which leads to (1), is valid for a long-range force such as the Coulomb force. Mapleton[3] has evaluated the Coulomb wave operator $\Omega^{(+)} = i\epsilon(E + i\epsilon - K - V)^{-1}$ by expanding it in Coulomb partial waves, and has shown that the function $\Omega^{(+)}\Phi_k$ differs from the usual Coulomb wave function by an energy-dependent factor. Previously, Okubu and Feldman[4] had studied the integral equation satisfied by $\Omega^{(+)}$ in momentum space, obtaining a similar result.

The T matrix, which is related to the wave operator by $T = V\Omega^{(+)}$, is thereby also in error.

Finally, one can show that the integral in (1), which has been evaluated for a Coulomb potential $V(r) = V_0/r$ by several authors,[5] does not lead to the correct Coulomb scattering amplitude. For if a convergence factor $e^{-\lambda r}$ is used in (1), the result is

$$(\mathbf{p}|T|\mathbf{k}) = \frac{V_0}{2\pi^2}C_0(\eta)e^{i\sigma_0}\lim_{\lambda \to 0}\frac{[p^2 - (k+i\lambda)^2]^{i\eta}}{[(\mathbf{p}-\mathbf{k})^2 + \lambda^2]^{1+i\eta}}, \qquad (2)$$

where

$$\eta = mV_0/\hbar^2 k,$$
$$C_0(\eta) = e^{-\pi\eta/2}|\Gamma(1+i\eta)|, \qquad (3)$$
$$\sigma_0 = \arg\Gamma(1+i\eta),$$

and the principal values of the powers are to be taken. If we now set $p = k$ and take the limit $\lambda \to 0$, the scattering amplitude, which is $-4\pi^2 m/\hbar^2$ times the T matrix, turns out to be

$$f_k(\hat{r}) = f_k{}^c(\hat{r})[\Gamma(1-i\eta)e^{-i\eta \ln(2k/\lambda)}], \qquad (4)$$

where $f_k{}^c(\hat{r})$ is the usual expression[6] for the Coulomb scattering amplitude:

$$f_k{}^c(\hat{r}) = -\frac{\eta}{2k \sin^2\frac{1}{2}\theta}e^{2i\sigma_0 - i\eta \ln(\sin^2\frac{1}{2}\theta)}. \qquad (5)$$

The squared modulus of the bracketed factor in Eq. (4) is $\pi\eta/\sinh(\pi\eta)$, similar to the extra factor found by Mapleton and by Okubu and Feldman. If the limit $\lambda \to 0$ is taken before setting $p = k$, an additional factor of

$$e^{\pm \pi\eta/2} \quad (p \lessgtr k) \qquad (6)$$

appears, so that (2) predicts a discontinuity at the energy shell as well as an incorrect scattering amplitude.

All of these difficulties seem to stem from the fact that the Coulomb potential distorts not only the scattered wave but also the incident plane wave. Thus, for

[1] T. Pradhan, Phys. Rev. 105, 1250 (1957); T. Pradhan and D. N. Tripathy, *ibid.* 130, 2317 (1963).

[2] R. Akerib and S. Borowitz, Phys. Rev. 122, 1177 (1961).

[3] Robert A. Mapleton, J. Math. Phys. 2, 482 (1961); 3, 297 (1962).

[4] Susumu Okubu and David Feldman, Phys. Rev. 117, 292 (1960).

[5] A. Nordsieck, Phys. Rev. 93, 785 (1954); T. Pradhan, *ibid.* 105, 1250 (1957).

[6] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), 2nd ed., pp. 114–120.

for which the $l=0$ radial wave function may be written in closed form:

$$F_0(kr) = NC_0(\eta)kRz\,_2F_1(1+i\alpha, 1-i\beta; 2; z)e^{ikr}, \quad (37)$$

$$z = 1 - e^{-r/R}, \quad (38)$$

$$\alpha = kR\{[1 + (2\eta/kR)]^{1/2} - 1\}, \quad \beta = \alpha + 2kR. \quad (39)$$

We assume R large enough that $|\eta/kR| \ll 1$; consequently, α is real.

The normalization constant N and the phase shift are determined as usual by the asymptotic form of $F_0(kr)$. This may be obtained by expanding the hypergeometric function about $z=1$, with the result that for $r \gg R$

$$F_0(kr) \sim NC_0(\eta)kR\left[\frac{\Gamma(i\beta - i\alpha)}{\Gamma(1-i\alpha)\Gamma(1+i\beta)}e^{ikr}\right.$$
$$\left. + \frac{\Gamma(i\alpha - i\beta)}{\Gamma(1+i\alpha)\Gamma(1-i\beta)}e^{-ikr}\right]. \quad (40)$$

Equation (40) may be written $F_0(kr) \sim \sin(kr + \delta_0)$ if we take

$$N = \frac{\beta}{2kRC_0(\eta)}\left|\frac{\Gamma(1+i\alpha)\Gamma(i\beta)}{\Gamma(i\beta - i\alpha)}\right| \quad (41)$$

and

$$\delta_0 = \arg\frac{\Gamma(1+i\alpha)\Gamma(i\beta - i\alpha)}{\Gamma(i\beta)}. \quad (42)$$

The case of interest is $R \to \infty$, so that $\alpha \to \eta$ and $\beta \to \infty$. We may therefore estimate the gamma functions by their asymptotic values, obtaining

$$\frac{\Gamma(i\beta - i\alpha)}{\Gamma(i\beta)} = \frac{\Gamma(2ikR)}{\Gamma(2ikR + i\alpha)} = (2ikR)^{-i\eta}\left[1 + O\left(\frac{\eta}{kR}\right)\right]; \quad (43)$$

the normalization constant and the phase shift then take on the familiar values

$$N \sim 1, \quad \delta_0 \sim \sigma_0 - \eta \ln(2kR). \quad (44)$$

It is also interesting to find the form of $F_0(kr)$ when $r \ll R$. Using the relationship

$$_2F_1(a, b; c; z) = {_1F_1}(a; c; bz)[1 + O(1/b)] \quad (45)$$

between ordinary and confluent hypergeometric functions, we may write

$$F_0(kr) = F_0{}^c(kr)[1 + O(r/R) + O(\eta/kR)], \quad (46)$$

a not unexpected result.

Let us turn now to the evaluation of $I(p)$, which in this case can be carried out exactly. After the variable of integration is changed to $z = 1 - \exp(-r/R)$, $I(p)$ becomes

$$I(p) = 2\eta kRNC_0(\eta)\int_0^1 (1-z)^{i\gamma}$$

$$_2F_1(1+i\alpha, 1-i\beta; 2; z)dz, \quad (47)$$

where

$$\gamma = (p - k)R. \quad (48)$$

This integral can be expressed[9] in terms of a generalized hypergeometric function:

$$I(p) = \frac{2\eta kRNC_0(\eta)}{1+i\gamma}\,_3F_2(1+i\alpha, 1-i\beta, 1; 2, 2+i\gamma; 1). \quad (49)$$

We may simplify Eq. (49) considerably by invoking the series definitions of the $_3F_2$ and $_2F_1$ functions and by using the fact that $(1+a)_n = (a)_{n+1}/a$.

$$I(p) = \frac{2\eta kRNC_0(\eta)}{1+i\gamma}\sum_{n=0}^{\infty}\frac{(1+i\alpha)_n(1-i\beta)_n}{(2+i\gamma)_n(n+1)!}$$

$$= \frac{2\eta kRNC_0(\eta)}{\alpha\beta}[_2F_1(i\alpha, -i\beta; 1+i\gamma; 1) - 1]$$

$$= NC_0(\eta)\left[\frac{\Gamma(1+i\gamma)\Gamma(1-i\alpha+i\beta+i\gamma)}{\Gamma(1-i\alpha+i\gamma)\Gamma(1+i\beta+i\gamma)} - 1\right]. \quad (50)$$

This expression is valid for all p. When $p = k$, $\gamma = 0$ and we get

$$I(k) = NC_0(\eta)\left[\frac{\Gamma(1-i\alpha+i\beta)}{\Gamma(1-i\alpha)\Gamma(1+i\beta)} - 1\right]$$
$$= e^{i\delta_0} - NC_0(\eta) \quad (51)$$

just as in Eq. (29); thus,

$$(k|T_0|k) = (e^{2i\delta_0} - 1)/2ik. \quad (52)$$

When $p \neq k$, both β and γ are large compared to α. Again using the asymptotic form of the gamma function, we obtain

$$I(p) = NC_0(\eta)[(1+i\gamma)^{i\eta}(1-i\alpha+i\beta+i\gamma)^{-i\eta} - 1]$$
$$+ O[\eta/(p-k)R]. \quad (53)$$

Our final expression for $(p|T_0|k)$ is then

$$(p|T_0|k) = \frac{C_0(\eta)e^{i\delta_0}}{2ip}\left[\left(\frac{p-k-i\lambda}{p+k-i\lambda}\right)^{i\eta} - \left(\frac{p+k+i\lambda}{p-k+i\lambda}\right)^{i\eta}\right]$$
$$+ O\left[\frac{\eta}{(p-k)R}\right], \quad (54)$$

where $\lambda = 1/R$. This agrees perfectly with the result of the previous section in the region where both are valid, i.e., $|p - k| \gg 1/R$.

V. DISCUSSION

The foregoing analysis can of course be extended to values of l beyond $l=0$, although results in closed form are possible only for the cutoff Coulomb potential. It

[9] *Tables of Integral Transforms*, Bateman Manuscript Project, edited by A. Erdélyi (McGraw-Hilll Book Company, Inc., New York, 1954), Vol. II, p. 399, Eq. (5).

is well known[10] that the phase shifts so obtained are given by

$$\delta_l \sim \sigma_l - \eta \ln(2kR), \qquad (55)$$

provided that $l \ll kR$. When $l \gg kR$, the phase shifts fall rapidly to zero because of the angular momentum barrier; the intermediate region $l \approx kR$ is quite hard to handle.

Under the assumption, however, that R is so large as to make contributions from $l \gtrsim kR$ generally negligible,[10] comparison of Eqs. (11) and (17) reveals that

$$\psi_k(\mathbf{r}) \cong e^{-i\eta \ln 2kR} \psi_k^c(\mathbf{r}), \quad r < R. \qquad (56)$$

The equality does not hold for $r > R$ because $\psi_k^c(\mathbf{r})$ has logarithmic distortions not possessed by $\psi_k(\mathbf{r})$.

Let us now assume that $(\mathbf{p}|T|\mathbf{k})$ is calculated as in the Introduction, but using Eq. (56), rather than just $\psi_k^c(\mathbf{r})$, as the approximation to $\psi_k(\mathbf{r})$. Quite obviously, the result is identical to Eq. (2), except that $e^{i\sigma_0}$ is replaced by $e^{i\delta_0}$:

$$(\mathbf{p}|T|\mathbf{k}) = \frac{V_0}{2\pi^2} C_0(\eta) e^{i\delta_0} \lim_{\lambda \to 0} \frac{[p^2 - (k+i\lambda)^2]^{i\eta}}{[(\mathbf{p}-\mathbf{k})^2 + \lambda^2]^{1+i\eta}}. \qquad (2')$$

If we now expand Eq. $(2')$ in Legendre polynomials according to Eq. (14), we find that

$$(p|T_l|k) = -\frac{\eta C_0(\eta) e^{i\delta_0}}{2p} \left[\frac{p^2 - (k+i\lambda)^2}{2pk} \right]^{i\eta} A_l(x), \qquad (57)$$

where

$$A_l(x) = \int_{-1}^{1} P_l(\mu)(x-\mu)^{-1-i\eta} d\mu \qquad (58)$$

and

$$x = (p^2 + k^2 + \lambda^2)/2pk. \qquad (59)$$

We are primarily concerned with the coefficient A_0, which is easily obtained:

$$A_0 = (1/i\eta)[(x-1)^{-i\eta} - (x+1)^{-i\eta}]. \qquad (60)$$

Thus, the $l=0$ component of Eq. $(2')$ is given by

$$(p|T_0|k) = \frac{C_0(\eta) e^{i\delta_0}}{2ip} \left[\left(\frac{p-k-i\lambda}{p+k-i\lambda} \right)^{i\eta} - \left(\frac{p+k+i\lambda}{p-k+i\lambda} \right)^{i\eta} \right]. \qquad (61)$$

This agrees with the results of Secs. III and IV when $p^2 \neq k^2$ both in magnitude and phase (the limit $\lambda \to 0$ is understood). If the calculations of Sec. III are repeated for higher values of l, one again finds agreement with Eq. (57) for $p^2 \neq k^2$. We are therefore led to the conclusion that the Coulomb T matrix does possess a discontinuity at the energy shell, and that furthermore the T matrix is correctly represented off the energy shell by Eq. (2), provided $e^{i\sigma_0}$ is replaced by $e^{i\delta_0}$.

It is not difficult to see why Eq. (1) gives incorrect results on the energy shell when the approximation (56) is used. In the first place the Coulomb potential is a long-range potential, even though a convergence factor is used. Hence, we may expect to get contributions from the asymptotic region of $\psi_k(\mathbf{r})$, where the approximation is not valid. However, because the rapidly oscillating factors, $e^{-i(p\pm k)r}$, appear after the angular integration, contributions from the asymptotic region are negligible unless $|p-k| \sim 1/R$. This is precisely the condition found in Secs. III and IV.

In summary, then, we have seen that the discontinuity in the T matrix found by Okubo and Feldman and by Mapleton is quite real,[11] and that off the energy shell Eq. (2) is essentially correct. Thus, Eq. (1), which is a valid definition of the T matrix for finite range forces, may also be used for the Coulomb force provided that shielding effects are taken into account when $p^2 = k^2$.

ACKNOWLEDGMENTS

APPENDIX: COULOMB SCATTERING AMPLITUDE

We have deliberately ignored the problem of evaluating $(\mathbf{p}|T|\mathbf{k})$ on the energy shell, or the equivalent problem of finding the screened Coulomb scattering amplitude in the limit of zero screening. The customary way of doing this is to look at the coefficient of e^{ikr}/r in the asymptotic expansion of Eq. (56). We have seen, however, that Eq. (56) is valid only when $r < R$; it cannot be used when r is much larger than the range of the force. On the other hand, the experimental situation, in which measurements are made by a detector located well outside the range of the force, clearly corresponds to $r \gg R$.

One may argue that, as long as $kr \gg \eta$, it does not matter much whether $r < R$ or $r > R$; the asymptotic form changes very little. This is probably true, but it would be nice to have a direct verification such as we have presented here for the T matrix off the energy shell. This involves performing the sum

$$\sum_l (2l+1) \frac{e^{2i\delta_l} - 1}{2ik} P_l(\cos\theta), \qquad (A1)$$

where, for $kR \ll l$,

$$\delta_l = \sigma_l - \eta \ln 2kR. \qquad (A2)$$

[Incidentally, we note that $\sigma_l \sim \eta \ln(l+1)$ for large l, so that the phase shifts δ_l approach zero as l approaches kR.]

At first we thought that Eq. (2) might have precisely

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[10] For a discussion, see G. Breit, Rev. Mod. Phys. **34**, 766 (1963), Sec. 4.

[11] It should be pointed out, however, that the T matrix obtained by these authors does not have the correct magnitude when $p^2 \neq k^2$, although the discontinuity is correctly given.

the correct angular dependence on the energy shell, in spite of the fact that its magnitude is clearly wrong. However, upon evaluating A_l for $p^2 = k^2$, we find[12]

$$A_l = (1/i\eta)(\lambda^2/2k^2)^{-i\eta}[{}_2F_1(-l, l+1; 1-i\eta; -\lambda^2/4k^2)$$
$$- (1+4k^2/\lambda^2)^{-i\eta}e^{2i(\sigma_l-\sigma_0)}$$
$$\times {}_2F_1(-l, l+1; 1+i\eta; -\lambda^2/4k^2)]$$
$$= -(1/i\eta)(\lambda^2/2k^2)^{-i\eta}[e^{2i(\delta_l-\sigma_0)}-1]+O(\eta/k^2R^2)$$
$$+O(l/k^2R^2), \quad (A3)$$

where as before $R=1/\lambda$. Thus, the expansion of Eq. (2) on the energy shell (with $e^{i\delta_0}$ replacing $e^{i\sigma_0}$) may be written

$$f_{\mathbf{k}}(\hat{r}) = \Gamma(1+i\eta)\sum_{l=0}^{L}(2l+1)\frac{e^{2i(\delta_l-\sigma_0)}-1}{2ik}P_l(\cos\theta)+\mathfrak{R}, \quad (A4)$$

where L is very large but satisfies $L \ll kR$, δ_l is given by Eq. (A2), terms of order η/kR have been ignored, and $\mathfrak{R}$ represents the rest of the series. It is evident that even apart from the factor $\Gamma(1+i\eta)$, the series in Eq. (A4) is different from that in (A1).

We could argue, as do Landau and Lifshitz,[8] that the quantity

$$\sum_{l=0}^{L}(2l+1)P_l(\cos\theta)$$

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[12] See Ref. 3 for one method of performing the integral.

approaches $2\delta(1-\cos\theta)$ as $L \to \infty$ and so is only important when $\theta \lesssim \epsilon \sim 1/L$. In that case, Eqs. (A1) and (A4) differ only by a factor of $\Gamma(1+i\eta)\exp(-2i\sigma_0) = \Gamma(1-i\eta)$ except at very small angles, provided that $\mathfrak{R}$ is negligible when $\theta > \epsilon$. [The factor $\Gamma(1-i\eta)$ has been noted previously; cf. Eq. (4).]

The above argument is not very satisfying, but since we have been unable to sum Eq. (A1), it will have to do. The prescription for obtaining the T matrix on the energy shell from Eq. (2) is then (1) replace $e^{i\sigma_0}$ by $e^{i\delta_0}$, (2) divide by $\Gamma(1-i\eta)$. This causes Eq. (4) to become

$$f_{\mathbf{k}}(\hat{r}) = f_{\mathbf{k}}{}^c(\hat{r})e^{-2i\eta \ln 2kR}, \quad (A5)$$

the extra factor of $\exp(-i\eta \ln 2kr)$ coming from step (1). Note that this expression for $f_{\mathbf{k}}(\hat{r})$ may also be obtained from the asymptotic form of Eq. (56) if $r=R$. Assuming the correctness of Eq. (A5), we may then list the behavior of $\lim_{R\to\infty}|(\mathbf{p}|T|\mathbf{k})|$ near the energy shell as follows:

$$\lim_{R\to\infty}|(\mathbf{p}|T|\mathbf{k})| = \frac{V_0}{2\pi^2}\frac{1}{(\mathbf{p}-\mathbf{k})^2}$$

$$\times \begin{Bmatrix} C_0(\eta) \\ 1 \\ e^{\pi\eta}C_0(\eta) \end{Bmatrix} \text{ for } \begin{Bmatrix} (p-k)\to 0^+ \\ p=k \\ (p-k)\to 0^- \end{Bmatrix}. \quad (A6)$$